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A preconditioning approach for improved estimation of sparse polynomial chaos expansions

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Abstract

Compressive sampling has been widely used for sparse polynomial chaos (PC) approximation of stochastic functions. The recovery accuracy of compressive sampling highly depends on the incoherence properties of the measurement matrix. In this paper, we consider preconditioning the underdetermined system of equations that is to be solved. Premultiplying a linear equation system by a non-singular matrix results in an equivalent equation system, but it can potentially improve the incoherence properties of the resulting preconditioned measurement matrix and lead to a better recovery accuracy. When measurements are noisy, however, preconditioning can also potentially result in a worse signal-to-noise ratio, thereby deteriorating recovery accuracy. In this work, we propose a preconditioning scheme that improves the incoherence properties of measurement matrix and at the same time prevents undesirable deterioration of signal-to-noise ratio. We provide theoretical motivations and numerical examples that demonstrate the promise of the proposed approach in improving the accuracy of estimated polynomial chaos expansions.

Keywords: Polynomial approximation; Compressive sampling; Polynomial chaos expansion; Preconditioning

1. Introduction

Reliable analysis of natural and engineered systems necessitates the understanding of how the system response or quantity of interest (QoI) depends on uncertain inputs. Uncertainty quantification (UQ) tackles these issues with efficient propagation of input uncertainties onto the QoI. This is typically done by building approximate surrogates that replace computationally expensive simulations. Surrogates approximate QoI as an analytical function of random inputs and facilitate quantifying parametric uncertainty. As a widely used spectral surrogate, the polynomial chaos expansion (PCE) uses orthogonal polynomials for the approximation of QoI. In order to construct PCEs, i.e., to determine the expansion coefficients corresponding to different polynomial bases, a widely used approach is stochastic collocation. This approach is advantageous particularly because it is nonintrusive and easy to implement by reusing legacy codes. Examples of stochastic collocation methods include spectral projection [1,2], sparse grid

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interpolation [3,4], and least squares [5,6]. The outstanding challenge is that the number of required sample points for accurate approximation of PCE surrogate increases drastically as the dimensionality of uncertain input increases [7,8].

Recently, motivated by the fact that approximated PCEs for many high dimensional problems could be sparse, i.e. QoI can be represented with only few terms when expanded into polynomial chaos basis, compressive sampling has been effectively used to approximate PCE coefficients using a small number of sampled simulations and has thus alleviated the dimensionality-related challenge [8–13]. The accuracy of sparse polynomial approximation heavily relies on incoherence properties of measurement matrix, which is a matrix that consists of evaluated polynomial bases at sample points. Most commonly, in standard sampling, samples are generated randomly from the probability distribution of random inputs. Recently, specialized sampling strategies have been proposed in order to improve the accuracy of sparse PCEs. In [14], it was proposed to draw samples from Chebyshev probability distribution to construct a sparse Legendre-based PCE. The theoretical and numerical results in [10] showed that Chebyshev sampling deteriorates the recovery accuracy in high dimensional problems. Drawing samples randomly from the tensor grid of Gaussian quadrature points was recommended in [9,15]. Although the results showed significant accuracy improvement in low-dimensional problems, the results underperformed or were close to standard sampling in high-dimensional problems. A sampling strategy that outperforms standard sampling in both low-dimensional high-order and high-dimensional low-order problems was proposed in [16], and was called the coherence-optimal sampling. In coherence-optimal sampling, samples are drawn from a measure that minimizes the (local) coherence of orthogonal polynomial system. In [11], a near-optimal sampling strategy was proposed, which further improved coherence-optimal sampling by subsampling a few samples from a large pool of coherence-optimal samples in such a way that the resulting measurement matrix will have better cross-correlation properties.

In this work, instead of relying on experimenting with sampling strategies to improve incoherence properties, we take an alternative approach and use a preconditioning scheme to enhance these properties. The term *preconditioning* has already been used in the sparse PCE literature to refer to a weight matrix that is added to preserve asymptotic orthogonality of basis functions when non-standard sampling distributions are used [14,16,17]. Specifically, this weight function is designed such that the product of weight matrix and measurement matrix is an orthogonal matrix for an asymptomatically large number of samples from the prescribed non-standard distribution. Therefore, by construction, these preconditioning matrices are associated with a specific sampling distributions and cannot be used for standard sampling approaches. To the best of our knowledge, the present work is the first attempt at preconditioning the underdetermined polynomial measurement matrix, regardless of the chosen sampling distribution, towards better incoherence properties. Therefore, our proposed approach, for the first time, allows for preconditioning also for cases where samples are drawn according to the distribution of random inputs.

When the target stochastic function is exactly sparse with respect to the truncated PC bases and measurements are noiseless, one can borrow methods for designing optimal projection (or sensing) matrix in signal processing applications [18,19] to precondition underdetermined equation systems. This is because both the preconditioning matrix and the projection matrix will appear in the same way in the coherence-based objective that one seeks to optimize. However, when truncation error or measurement noise is present, that resemblance no longer exists. Therefore, in these polynomial regression problems, an improper design of preconditioning matrix can undesirably amplify the noise vector more than it does the measurement vector. This can result in a worse "signal-to-noise" ratio leading to inaccurate polynomial approximation.

In this work, we propose an original approach for designing the preconditioning matrix such that (1) the incoherence properties of the resulting preconditioned measurement matrix are improved, and (2) undesirable amplification of noise vector vis-á-vis measurement vector is prevented. The proposed preconditioning technique is also capable of preconditioning a system with no measurement or truncation error, and as such has general applicability. Using numerical examples, it will be demonstrated that preconditioning can significantly improve the accuracy of PCE surrogates built using compressive sampling. This paper is organized as follows: Section 2 provides a brief overview on application of compressive sampling in PCE approximation; Section 3 introduces the preconditioning scheme along with the theoretical motivation, and Section 4 includes numerical illustration and detailed discussion about the comparative performance of the proposed preconditioning scheme.

2. Setup and background

2.1. Polynomial chaos expansion

Consider the vector of independent random variables $\Xi = (\Xi_1, \ldots, \Xi_d)$ to be d-dimensional system random inputs and $u(\Xi)$ to be the uncertain QoI with finite variance. Then, $u(\Xi)$ can be written as an expansion of orthogonal